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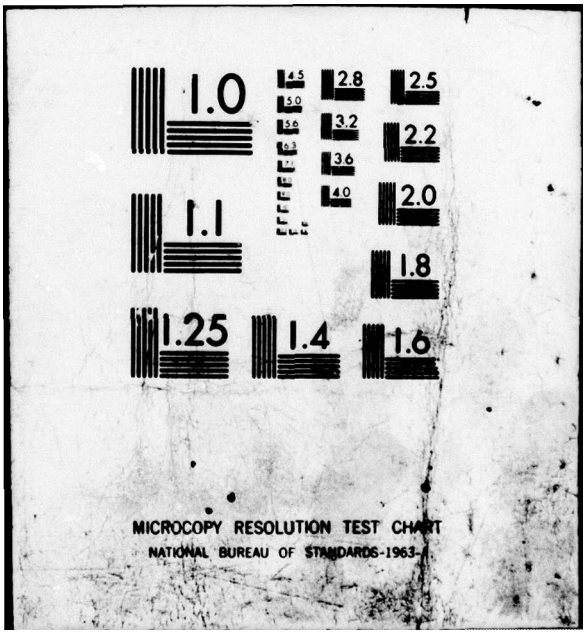
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QUANTUM FIELD THEORY METHODS APPLIED TO THE PHYSICS OF CONDENSED MATTER

FINAL REPORT

S. DONIACH

9 August 1979

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report summarizes briefly research performed under the grant. A complete list of Ph.D.'s awarded and associated researchers working with total or partial support is included. The report contains a full list of publications resulting from the research.

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1. Introduction

The principal thrust of the proposal on which this research grant was based was a study of mixed valence compounds. These are metallic materials in which the conduction electrons appear to resonate between fairly broadband states and very narrow, possibly localized, f-states. They are of particular interest since the time of resonance between these two kinds of states is within the range of many laboratory experiments — expressed in temperature units, $\hbar/\tau$ is of the order of 50-100°K.

As part of the proposal, it was suggested that one method which was needed to treat problems of this type would be an extension of the renormalization group method developed by K. Wilson for the Kondo problem, in which a single atom impurity in a host lattice of normal metallic character has a magnetic electron which interacts in a singular way with the electron gas of the metal.

Along with the development of suitable renormalization group methods, it was proposed to investigate the theory of other systems of restricted dimensionality — one and two dimensions, where these methods might be useful.

In this final report, the results obtained, supported wholly or partly by this grant, are briefly summarized.

A. The Kondo Lattice and Real Space Renormalization Group for Quantum Systems.

A very striking property of many mixed valence compounds is the fact that they have extremely anomalous magnetic behavior. Thus, for instance, $CeAl_3$ appears to be the metallic system with a non-magnetic ground state, even though evidence based on magnetic susceptibility and volume of the unit cell indicate that the f-level of cerium contains of the order of one electron. The investigator was one of the first to emphasize the anomalous magnetic character of this class of materials. He proposed[5] that this behavior might be understood on the basis of an extension of the properties of the Kondo model for a single impurity to those of an entire lattice of magnetic atoms interacting with an electron gas. The investigator gave the name "Kondo lattice" to this system, and this nomenclature has since become part of the technical language applied to this class of problems.

The quantum mechanical description of a non-magnetic ground state of a system containing a periodic array of magnetic centers presents a difficult mathematical problem. In some senses it may be said that it has not yet been solved in a satisfactory way. The investigator proposed the study of an extremely over-simplified model, consisting of a one-dimensional chain of localized magnetic electrons interacting with a 1-D chain of pseudo-spins, representing magnetic degrees of freedom of 1-D Fermi gas — this model was named the "Kondo necklace model".[5,6] Through the work of visiting Research Associate, R. Jullien, and graduate student, J. Fields, the properties of this model were investigated by means of a renormalization group technique, applicable to 1-D quantum systems.[7,8] This technique had been proposed earlier by Pearson and developed by Weinstein, Drell and Yankelowitz,* and by Scalapino, Stokely and Jafarey,† for the simpler problem of an Ising chain in a transverse magnetic field. The latter is one of the simplest 1-D cooperative problems which exhibits a critical point at zero temperature as a function of the ratio of the applied magnetic field to the exchange interaction.

The more complicated problem of the Kondo necklace was treated approximately by the technique, and it was shown that, indeed, the ground state does undergo spontaneous change of symmetry as a function of the Kondo coupling

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*S.D. Drell, M. Weinstein, and S. Yankielovicz, Phy. Rev. D14, (1976) 487.

†S. Jafarey, R. Pearson, D. Scalapino, and B. Stoeckley, (unpublished).

constant at zero temperature.[7,8] This result substantiated results obtained by the investigator on the basis of cruder approximations of the mean field type.[5,6]

Unfortunately, the Kondo necklace model is too simple to describe the full physics of the Kondo-lattice problem. A more recent investigation by Jullien *et al.*[16] has shown that similar properties may be expected for more realistic problems in which both spin and charge degrees of freedom of the 1-D electron gas are included.

At the same time as studying the Kondo necklace problem, Jullien, together with the investigator and other collaborators[18] has considerably extended the techniques of calculation needed for the quantum renormalization group and have applied it to studying the behavior of correlation functions and other critical exponents for the transverse Ising model. In publication 18, these results were found to compare rather favorably with the results of an exact solution for the 1-D transverse Ising model which had been obtained some years ago by Pfeuty.

B. Investigation of the Theory of Cooperative Systems of Reduced Dimensionality.

Along with the study of the renomalization group for quantum mechanical systems, the investigator also applied other techniques to the study of systems of reduced dimensionality.

Work with E. Rezayi focused on the study of the effect of the electron-phonon interaction on the interacting electron gas in 1-D. Such systems are of interest in connection with conductivity in organic semi-metals of the type TTF-TCNQ. Rezayi's work focused on the use of perturbative methods to study the renormalization-group equations for the electron-phonon interaction in 1-D systems. Such equations have been developed by Solyom *et al.* for the problem of the electron gas interacting through instantaneous (i.e., Coulomb) as opposed to retarded potentials. In the weak coupling limit, the work of Rezayi and the investigator has shown that the crossover from a superconducting (BCS type) ground state to a charge-density wave (Peierls) ground state is qualitatively changed by the presence of retardation (see publication 29 and Rezayi's Ph.D. thesis, Stanford, 1979).

Work by L. Turkevich and R. Klemm[24] investigated the effects of inter-chain coupling in 1-D superconducting chains, represented by a Ginzburg-Landau free-energy function. In this work, the anomalous properties of the critical pair-breaking magnetic field (H_{c_2}) as a function of the angle between the field and the chain direction were investigated in considerable mathematical detail.

Work by Turkevich and Doniach[25] has focused on the effect of the periodicity of the underlying atomic lattice structure on the free energy of a charge density wave system in one dimension. Using a Ginzburg-Landau free-energy functional approach, the cross over from the behaior of a charge density wave whose phase is free to vary between zero and 2π to that of a charge density wave which has become commensurate with the underlying lattice was studied as a function of the commensuration coupling constant and the temperature of the system. For this system the transfer matrix becomes a one-dimensional sine-Gordon equation which was studied in considerable mathematical detail. This system, although simpler than the 2-D sine-Gordon equation (one space, one time), nevertheless presents fairly formidable mathematical problems, which had been partially solved by Gupta and Sutherland. The work of Turkevich and Doniach extends this earlier study to the full range of coupling constants, i.e., both the incommensurate and commensurate phases, in the low-temperature regime.

In another study, Huberman, Meyerson and Doniach extended earlier ideas, due to Doniach, on the behavior of superfluid helium in thin films of thickness of the order of a few atomic spacings, by the application of the theory of Kosterlitz and Thouless to discuss the mechanism of dissipation of superflow in thin superfluid films. In this approach the kinetics of thermally excited pairs of quantum vortices are used to calculate the rate of dissipation of superflow.[17]

C. Application of Renormalization Group Techniques to Critical Dynamics

Research Associate, Mike Nolan, working in collaboration with G. Mazenko (University of Chicago) and O. Valls (University of Minnesota), has applied renormalization group techniques to the study of critical dynamics for systems of low dimensionality. The real space renormalization group (RSRG) had, until very recently, only been used to study static problems. A major research effort has now successfully culminated in the extension of the real space renormalization group to include dynamic problems.[21, 26, 27]

The formalism of the dynamic RSRG, which is quite general in nature, has been applied to the kinetic Ising models. Dynamic scaling exponents have been calculated for several different models in perturbation theory with results that compare quite favorably to expected values.

Current work also includes the calculation of dynamic correlation functions for the kinetic Ising models and the extensions of these methods to include systems with continuous rather than discrete symmetries. Also under consideration are a variety of "coarse graining" problems. The systematic relation between microscopic and hydrodynamic or macroscopic description for a variety of systems is poorly understood.

D. Theory of Sound Attenuation and Dispersion Near Critical Points

In previous work[22] it was shown that sound attenuation and dispersion in liquid-gas systems near the critical point are related to a certain four-point dynamic order parameter correlation function. While a simple 1/n expansion for this correlation function yielded results which compared much more favorably with experiment than did existing theories, it was thought that a more systematic evaluation of the correlation function would further improve the comparison between theory and experiment.

Using the momentum space renormalization group and memory function technique, a consistent first order in ϵ ($d=4-\epsilon$, where d is the dimensionality of the system) expansion was derived by M. Nolan for the four-point function. This expansion gives rise to an integral equation which must be inverted to explicitly calculate the sound attenuation and dispersion. A variety of analytical and computer techniques have been applied to the inversion of this integral equation. It is anticipated that the results will be written up for publication in the near future.

E. Graduate Students Supported by the Grant

The following students obtained Ph.D.'s on research partly supported by the grant:

Joseph Fields III,	Ph.D., 1978
Edward H.-Rezayi,	Ph.D., 1979
Lee Turkevich,	Ph.D., 1979

The following graduate students were supported by the grant; date of expectation of Ph.D. is in parenthesis:

Dana Browne	(1981)
Stuart Trugman	(1981).

F. Research Associates and Visitors Supported Wholly or Partly by the Grant

Prof. Karl-Frederick Berggren, Linköping University, Sweden
Dr. Bernard Caroli, University of Paris VII, France
Dr. Christianne Caroli, University of Paris VII, France
Dr. Duncan Haldane, Institute Laue-Langevin, Grenoble, France
Dr. Remi Jullien, University of Paris, South, Orsay, France
Prof. Richard Klemm, Iowa State University
Dr. Pascal Lederer, C.B.P.F., Brazil
Dr. Calagero Natoli, Laboratorio Nazionali Frascati, Italy
Dr. Erio Tosatti, International Centre di Teoretici Physica, Trieste, Italy

Dr. Michael J. Nolan, Stanford University

APPENDIX

List of Publications of Work Performed with Partial or Total Support by Army Durham on the Grant

1. S. Doniach, "High Energy Excitations in Molecules and Solids," in *Photoionization and Other Probes of Many-Electron Interactions*", ed. F.J. Wuillemier, Plenum Press, New York, 1976, 335.
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4. M.T. Beal Monad and S. Doniach, "The Possibility of Surface Ferromagnetism of Liquid He^3 in Confined Geometries," J. Low Temp. Phys. 28 185 (1977).
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9. E. Tosatti, W. Andreotti, M. DeCrescenzi, "Surface Effects in the Ultra-Violet Reflectance of Excitons in Solid Rare Gases," *Proceedings of the Montpelier Vacuum Ultraviolet Conference* (1977).
10. E. Tosatti and W. Andreotti,"Electronic Structure of Surface Vacancies on Si(111)," *Proceedings, Third International Conference on Solid Surfaces*, Vienna, 1977.
11. N.O. Lipari, M. Altarelli, and E. Tosatti, "Interpretation of Far-Infrared Absorption Spectra in Germanium", Solid State Communications (1977)
12. E. Tosatti, "Splitting of Anisotropic Excitons", Solid State Comms. (1977).
13. P.A. Lee, T.M. Rice and R.A. Klemm, "Role of Interchain Coupling in Linear Conductors," Phys. Rev. B15, (1977) 2984.

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15. A. Caille, A. Rapini, S. Doniach, M. Zuckerman, and A. Gros, "A Simple Model for Phase Transitions in Monolayers and Bilayers of Lipid Molecules," Canadian J. of Physics, 56, (1978) 348.

16. R.Jullien, P. Pfeuty, J.N. Fields and S. Doniach, "Theoretical Study of the Kondo Lattice", Proceedings of the Conference on Rare Earth and Actinide Compounds, St. Remi La Chevreuse, 1979.

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24. L. Turkevich and R. Klemm, "Ginzburg Landau Theory of the Upper Critical Field in Filamentary Superconductors," Phys. Rev. B18, (1979) ...

25. L. Turkevich and S. Doniach, "Commensurate and Incommensurate Transitions in Pseudo-One-Dimensional Ginzburg-Landau Systems," in preparation

26. G.F. Mazenko, M.J. Nolan, and O.T. Valls, "The Real Space Dynamic Renormalization Group, I.: General Formalism," submitted for publication.

27. G. F. Mazenko, M.J. Nolan, and O.T. Valls, "The Real Space Dynamic Renormalization Group, II: Simple Examples," submitted for publication.

28. E. Rezayi, "Green's Function Theory of Extended X-Ray Absorption Fine Structure" Structure," Stanford Synchrotron Radiation Laboratory Reprt, 1979.

29. E. Rezayi and S. Doniach, "Effect of Electron Phonon Interaction on the Instabilities of a 1-dimensional Electron Gas", (in preparation).